Ecotox Report for Case # P-18-0116

General

[redacted]

Report Status: Complete
Status Date: 10/04/2018
CRSS Date: 03/05/2018
SAT Date: 03/06/2018
SAT Chair: William Irwin
Consolidated PMN: N
Consolidated Set:
Ecotox Related Cases: [redacted]
Health Related Cases:
Submitter: [redacted]
CAS Number: 1186514-12-4
Chemical Name: Castor oil, reaction products with soybean oil
Use: [redacted]
Trade Name: [redacted]
PV-max(kg/yr): [redacted]
Ecotox Assessor: Muneer, Alie

Fate Summary Statement

Fate Summary Statement: P-18-0116

FATE: [redacted]

Liquid with MP [redacted]
log Kow = [redacted]

H < 1.00E-8 (E)
log Koc = 3.23 (E)
log Fish BCF = 1.50 (32)

(E)
log Fish BAF = 1.17 (15) (E)
POTW removal (%) = 90 via
sorption and biodeg; OECD 301F(Mano Resp): 72%/28d, NRB;
MSDS (no
study report, inherent biodegradation): 78%/28d.
Time for complete
ultimate aerobic biodeg = wk
Sorption to soils/sediments = moderate

PBT Potential: P2B1
*CEB FATE: Migration to ground water = slow

Bioconcentration factor to be put into E-FAST: 15

PMN
Material:
Overall wastewater treatment removal is 90% via sorption and biodegradation.
Sorption to sludge is strong based on the estimated physical-chemical properties from EPISUITE.
Air Stripping
(Volatilization to air) is negligible based on the estimated physical-chemical properties from EPISUITE.
Removal by
biodegradation in wastewater treatment is high based on measured data for the PMN substance (OECD 301F (Mano Resp): [redacted]

Destruction of the substance in wastewater treatment is complete based on measured data for the PMN substance (OECD 301F (Mano Resp): [redacted]
The aerobic aquatic biodegradation
half-life is weeks based on measured data for the PMN substance (OECD 301F
(Mano Resp): [redacted]
The anaerobic aquatic
biodegradation half-life is months based on the estimated aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life.
Sorption to soil and sediment is moderate based

on the estimated physical-chemical properties from EPISUITE.

Migration to groundwater is slow, mitigated by biodegradation.

PMN Material:
Moderate Persistence (P2) is based on the aerobic
and anaerobic biodegradation half-life.
Low Bioaccumulation
potential (B1) is based on BCFBAF model estimates.

Bioconcentration/Bioaccumulation factor to be put into E-Fast:
15.

Physical Chemical Information

Molecular Weight:	[redacted]		
Wt% < 500:		**Wt% < 1000:**	
Physical State - Neat:	Liquid		
Melting Point:	[redacted]	**Melting Point (est):**	
MP (EPI):	[redacted]		
Vapor Pressure:		**Vapor Pressure (est):**	[redacted]
VP (EPI):	[redacted]		
Water Solubility:	[redacted]	**Water Solubility (est):**	
Water Solubility (EPI):			
Henry's Law::			
Log Koc:		**Log Koc (EPI):**	
Log Kow:		**Log Kow (EPI):**	[redacted]
Log Kow Comment:			

SAT Concern Level

Ecotox Rating (1):	3
Ecotox Rating Comment (1):	

Ecotox Rating (2):	
Ecotox Rating Comment (2):	
Ecotox Route of Exposure:	All releases to water

Ecotox Comments

Exposure Based Review (Eco):	N
Ecotox Comments:	
Exposure Based Testing:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
2	1	1	

Eco-Toxicity Comment:

Fate Ratings

Removal in WWT/POTW (Overall): 90

Condition	Rating Values	Rating Description 1	2	3	4	Comment
Fish BCF:						
Log Fish BCF:						
WWT/POTW Sorption:	3	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	2	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:	2	Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	2	<= Days	Weeks	Months	> Months	

Removal in WWT/POTW (Overall):	90					
Condition	**Rating Values**	**Rating Description** **1**	**2**	**3**	**4**	**Comment**
Aerobic Biodeg Prim:	2	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	3	<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Prim:	3	<= Days	Weeks	Months	> Months	
Hydrolysis (t1/2 at pH 7,25C) A:	3	<= Minutes	Hours	Days	>= Months	
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months	
Sorption to Soils/Sediments:	3	V. Strong	Strong	Moderate	Low	
Migration to Ground Water:	2	Negligible	Slow	Moderate	Rapid	
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid	
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid	
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid	

Bio Comments: PMN Material:
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Removal by biodegradation in wastewater treatment is high based on measured data for the PMN substance (OECD 301F (Mano Resp): [redacted]

Destruction of the substance in wastewater treatment is complete based

Removal in WWT/POTW (Overall):	90					
Condition	**Rating Values**	**Rating Description** 1	2	3	4	**Comment**
		on measured data for the PMN substance (OECD 301F (Mano Resp): [redacted] The aerobic aquatic biodegradation half-life is weeks based on measured data for the PMN substance (OECD 301F (Mano Resp): [redacted] The anaerobic aquatic biodegradation half-life is months based on the estimated aerobic biodegradation half-life. The anaerobic biodegradation half-life is projected to be greater than or equal to the aerobic biodegradation half-life. Sorption to soil and sediment is moderate based on the estimated physical-chemical properties from EPISUITE. Migration to groundwater is slow, mitigated by biodegradation. PMN Material: Moderate Persistence (P2) is based on the aerobic and anaerobic biodegradation half-life. Low Bioaccumulation potential (B1) is based on BCFBAF model estimates. Bioconcentration/Bioaccumulation factor to be put into E-Fast: 15.				
Fate Comments:		PMN Material: Overall wastewater treatment removal is 90% via sorption and biodegradation. Sorption to sludge is strong based on the estimated physical-chemical properties from EPISUITE. Air Stripping (Volatilization to air) is negligible based on the estimated physical-chemical properties from EPISUITE. Removal by biodegradation in wastewater treatment is high based on measured data for the PMN substance (OECD 301F (Mano Resp): [redacted]				

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Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	96-h	LC50	1.1	>100	P: LMW monoester M: WAF
Daphnid	48-h	LC50	1.6		""
Green Algae	96-h	EC50	0.44	>100	""
Fish	-	Chronic Value	0.04		

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
					P: LMW monoester
Daphnid	-	Chronic Value	0.49		P: LMW monoester
Green Algae	-	Chronic Value	0.28	100	P: LMW monoester M: WAF (NOEC)

Ecotox Value Comments: Predictions are based on the LMW monoester and QSARs for [redacted] (ECOSAR V2.0); [redacted] effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO3; and TOC <2.0 mg/L.

Background:
The sponsor, [redacted] has submitted test data for a 96-hr acute fish toxicity test, 48-hr acute daphnid toxicity test, and 72-hr acute algae toxicity test conducted for the PMN substance.

The PMN substance is a neat liquid, low bioaccumulation concern, slightly soluble in water, and nonvolatile in water. [redacted] The physical state for end use is destroyed. The physical and chemical properties for the PMN substance include the following estimated values from [redacted]

Fish Ecotoxicity Test:

[redacted]

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
[redacted]					

solubility)

Daphnid Ecotoxicity Test:

[redacted]

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
[redacted]					

Algal Ecotoxicity Test:

[redacted]

Conclusion:
All acute toxicity tests are not acceptable and

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
					therefore the acute and chronic COCs are based on predicted values from ECOSAR Esters-poly chemical class. For all acute toxicity tests, testing was conducted above the water solubility. [redacted] Analytical techniques should have tested below the water solubility concentration of [redacted] A range finding study around the measured water solubility value of [redacted] should have been performed and was not performed for all acute toxicity studies. The filter pore size of [redacted] was acceptable for all acute toxicity studies. Based on predicted values from ECOSAR for esters-poly chemical class, the acute COC is 110 ppb and chronic COC is 4 ppb. Acute COC: 110 ppb based on predicted values from ECOSAR esters-poly chemical class Chronic COC: 4 ppb based on predicted values from ECOSAR esters-poly chemical class Ecotox Reviewer: Alie Muneer Date: March 15, 2018

Ecotox Factors

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic (ppb):		4/10	110	
Chronic Aquatic (ppb):			4	

Factors	Values	Comments
SARs:	Esters	
SAR Class:	Esters-poly	
TSCA NCC Category?	Esters	

Recommended Testing:	
Ecotox Factors Comments:	Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risks because the significance of the risk is

dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model (https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model)
and hazard data on analogous chemicals. Based on these estimated hazard values from ECOSAR and hazard data on analogous chemicals, EPA concludes
that this chemical substance is a high environmental hazard.

.
Substance falls within the TSCA New Chemicals Category of Esters.
·
ECOSAR chemical class of Esters-poly.
· High hazard based on an acute
COC of 110 ppb and chronic COC of 4 ppb base on predicted values from ECOSAR chemical class Esters, based on the LMW monoester, which is the smallest chemical structure (i.e., it's the top left chemical
structure.)

Environmental Risks:
-Risks were not identified for
ecotoxicity

Potentially Useful Information:
Aquatic
Toxicity

Comments/Telephone Log

Artifact	Update/Upload Time
[redacted]	02/28/2018 08:01